

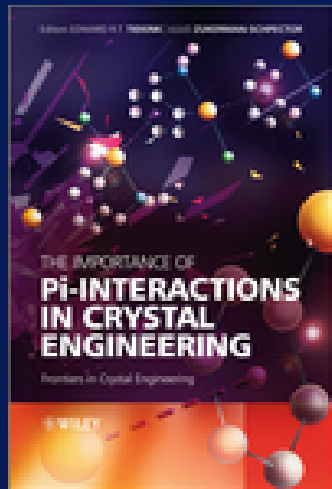


An analysis of chloride... π (chelate ring) interactions

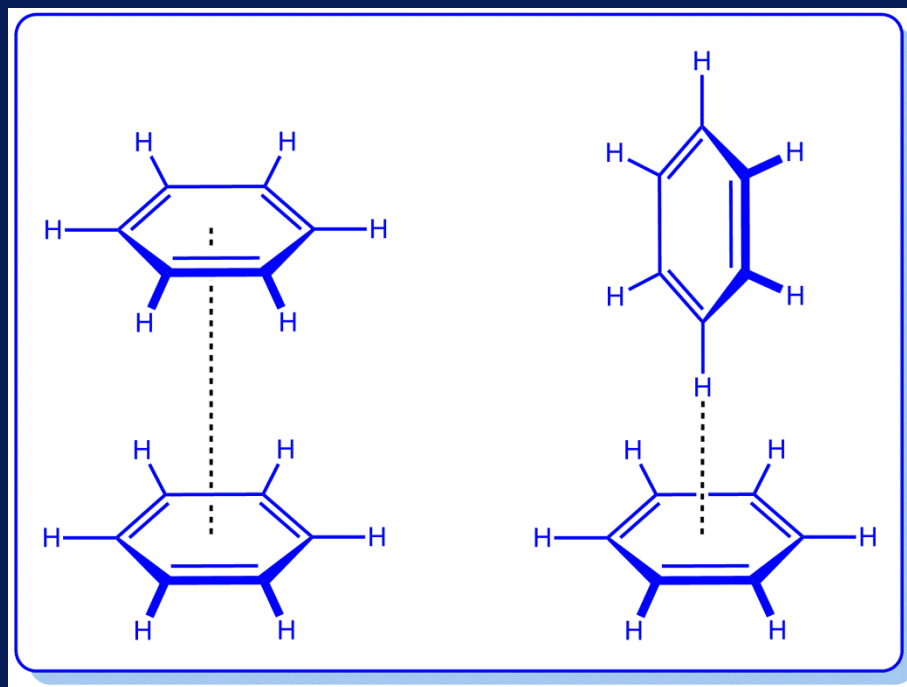
Edward R.T. Tiekink
Research Centre for Crystalline Materials



π -Systems in Supramolecular Chemistry

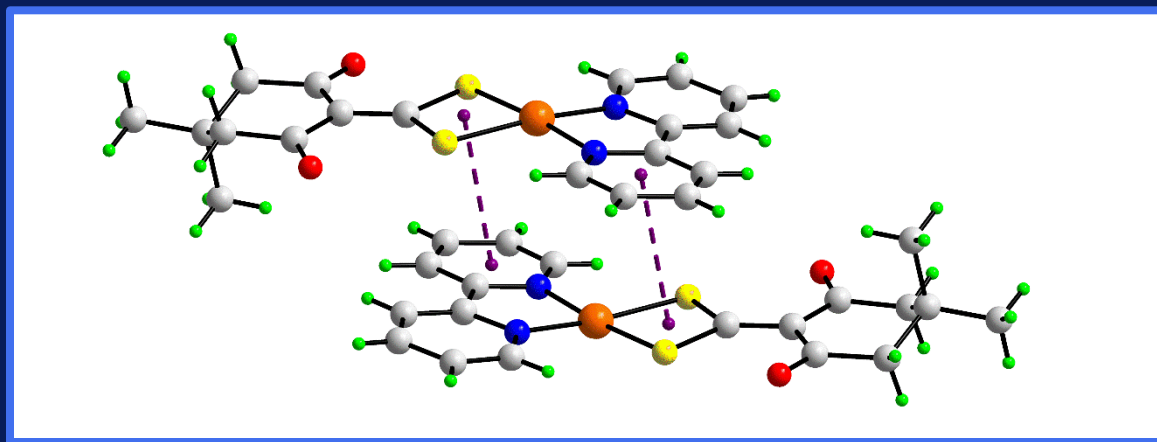


Classic π -systems/interactions

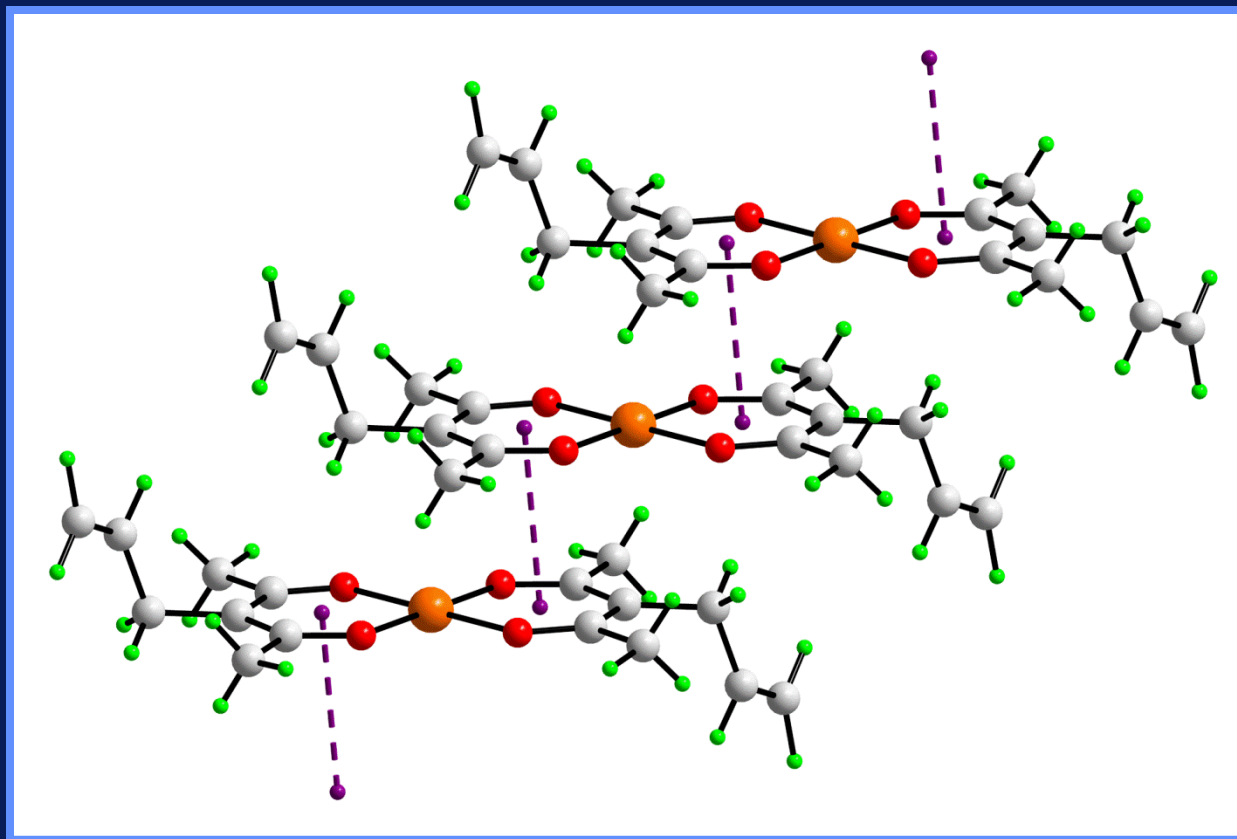


face-to-face edge-to-face

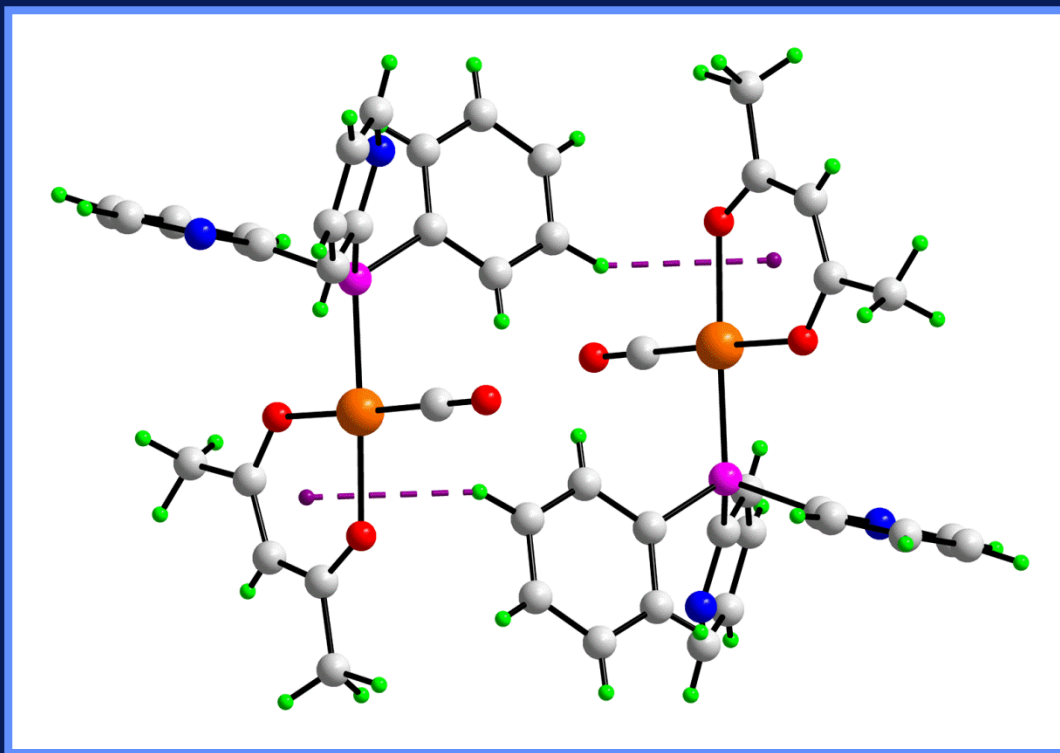
Intermolecular interactions involving chelate rings



Intermolecular interactions involving chelate rings



Intermolecular interactions involving chelate rings



$\pi\cdots\pi$ (chelate) interactions

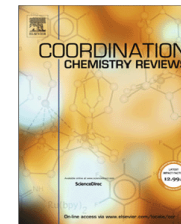
Coordination Chemistry Reviews 345 (2017) 318–341



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Review

Noncovalent bonding: Stacking interactions of chelate rings of transition metal complexes



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^a Department of Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia

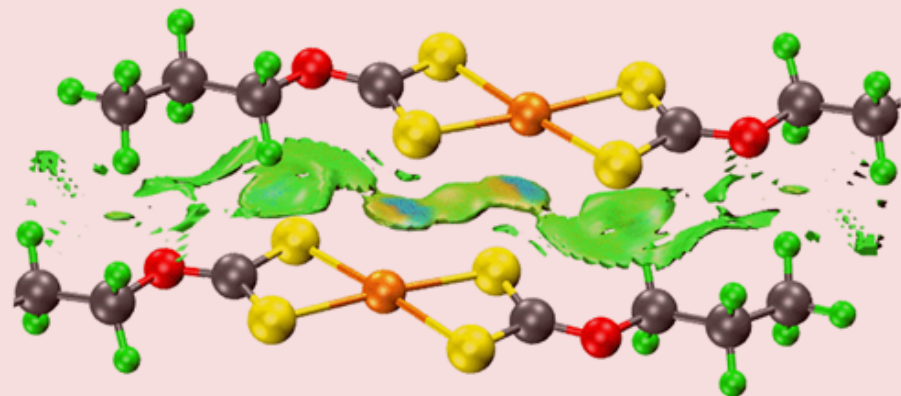
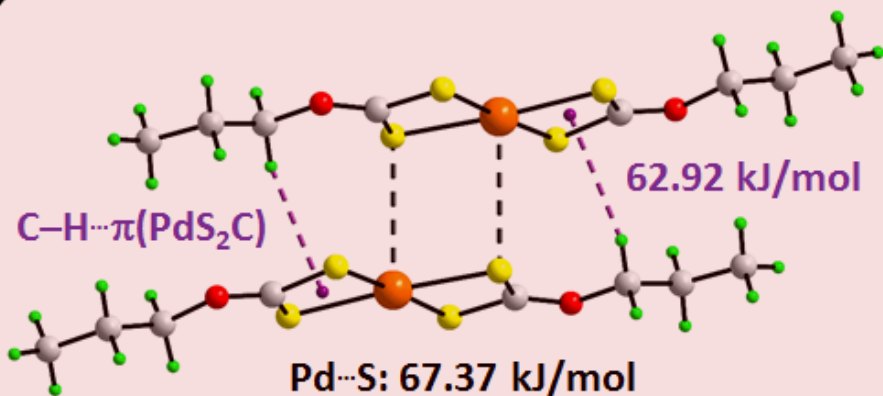
^b Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11001 Belgrade, Serbia

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^d Department of Chemistry, Texas A&M University at Qatar, P. O. Box 23874, Doha, Qatar

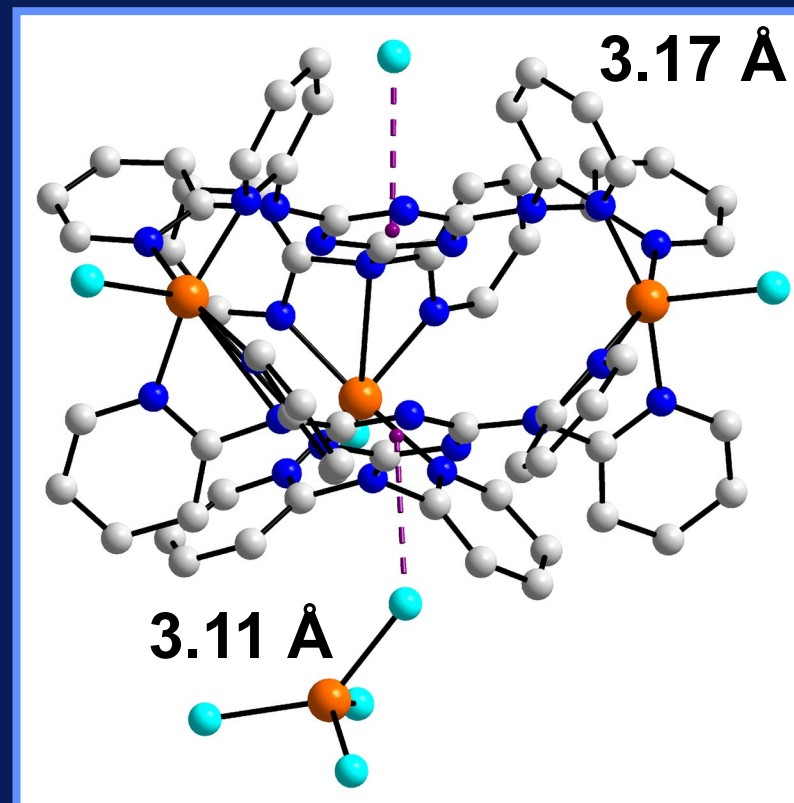
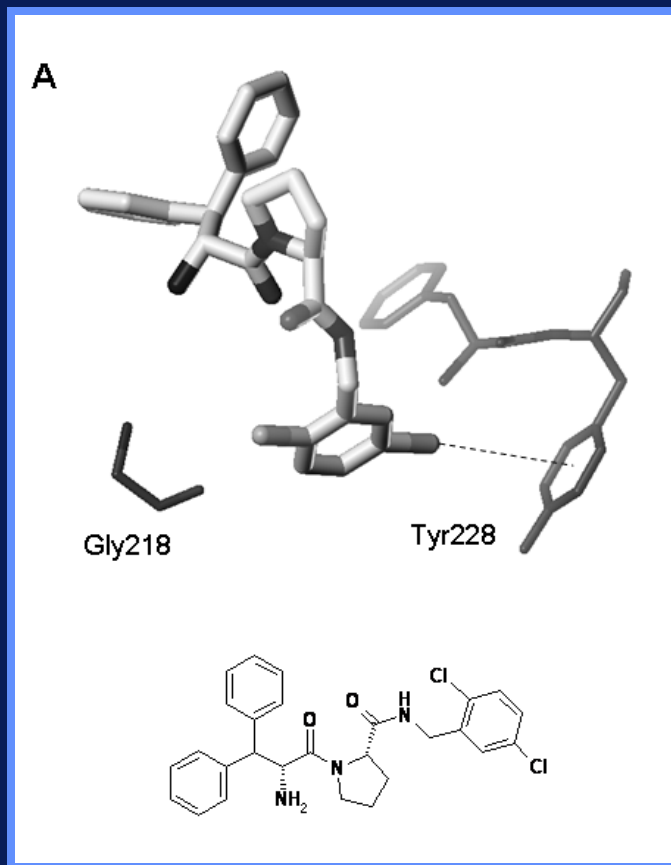


C-H... π (chelate ring)



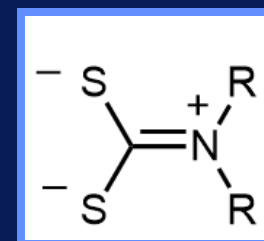
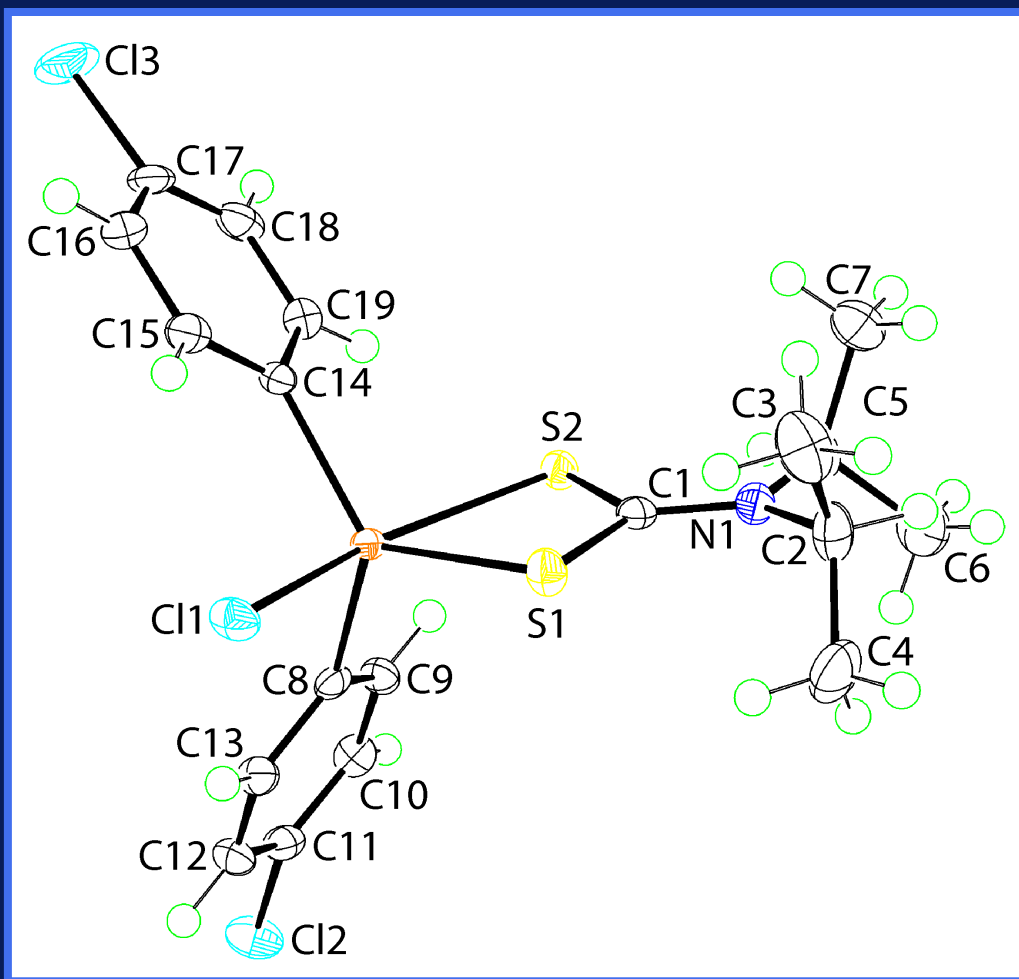
Pd...S	16 kcal/mol
C-H... π (chelate)	15 kcal/mol

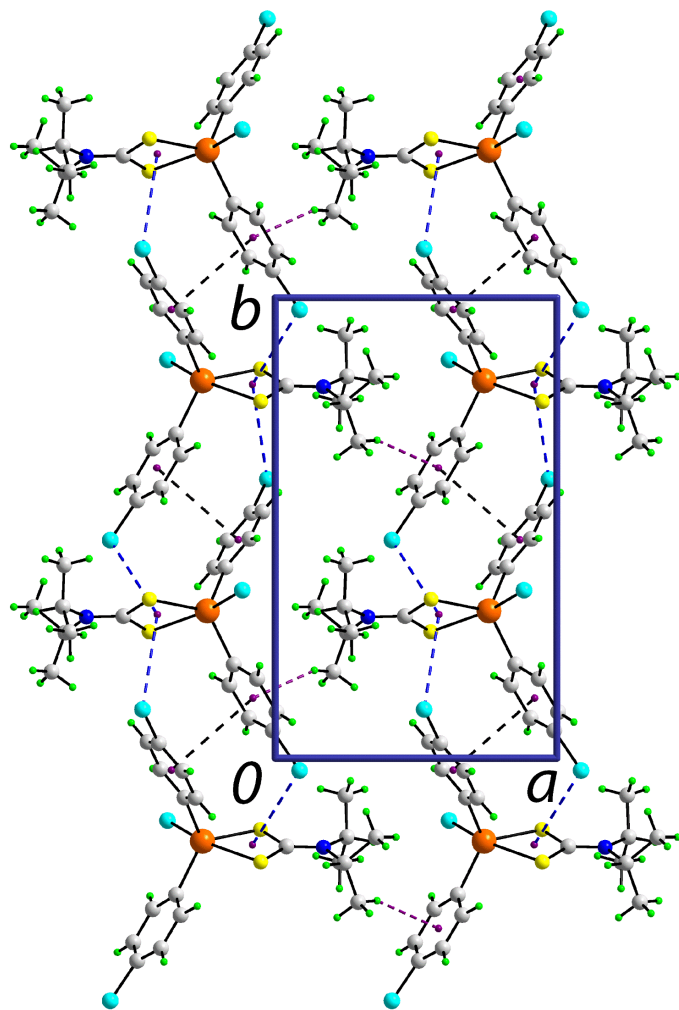
C-Cl $\cdots\pi$ (arene) interactions



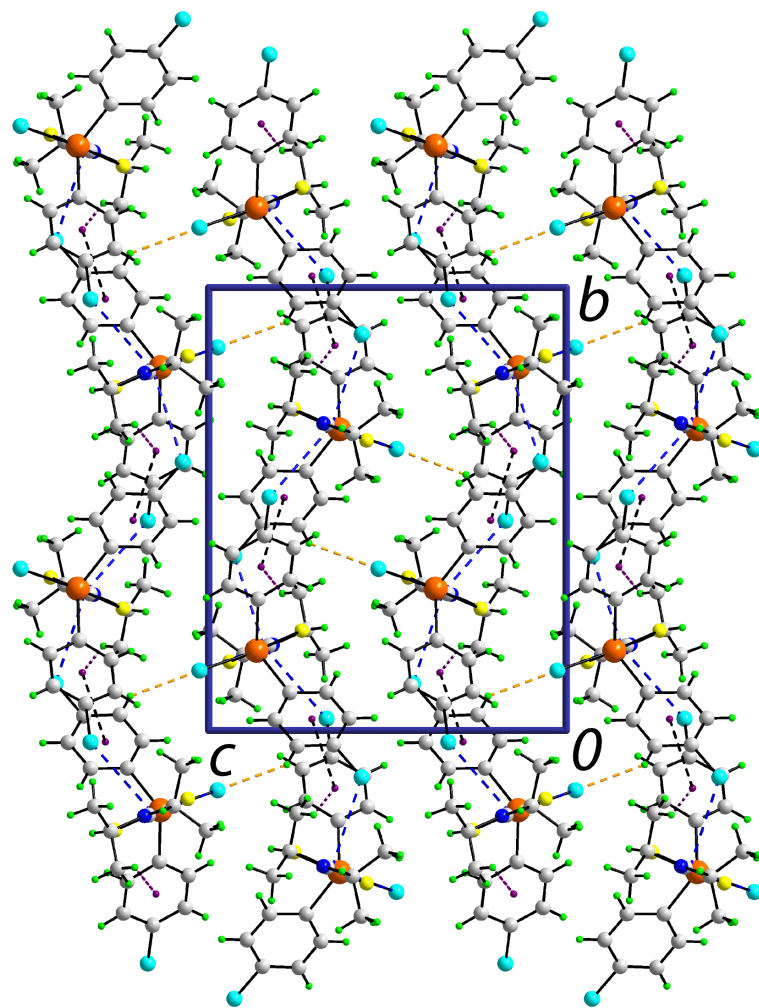
Tucker et al., *J. Med. Chem.*, **1998**, 41, 3210–3219.

Demeshko et al., *J. Am. Chem. Soc.*, **2004**, 126, 4508–4509.

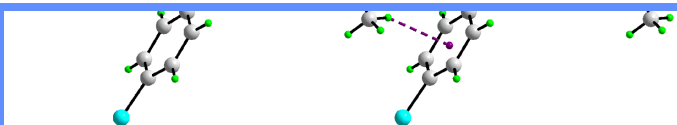
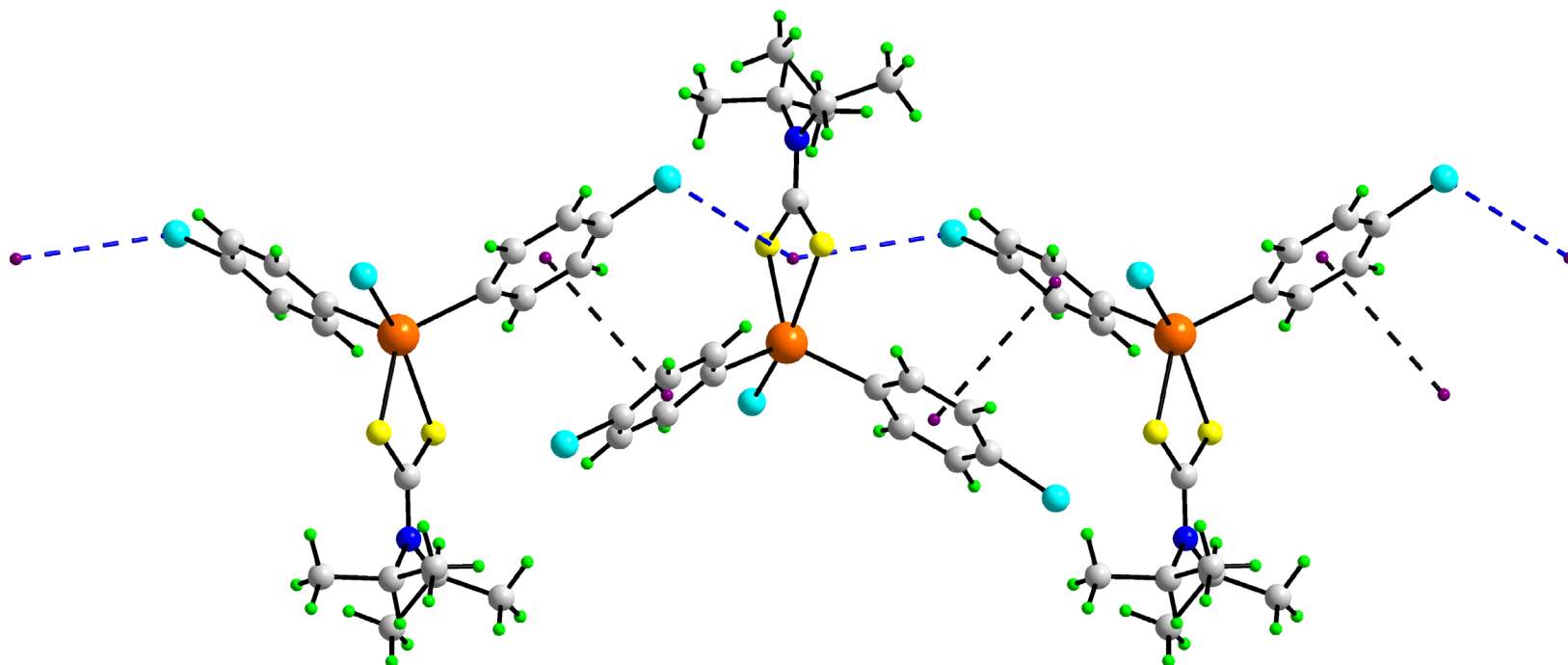




(a)

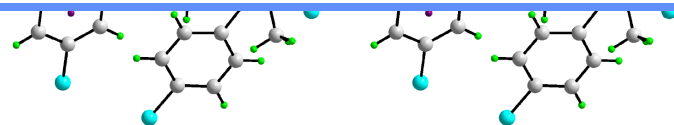


(b)

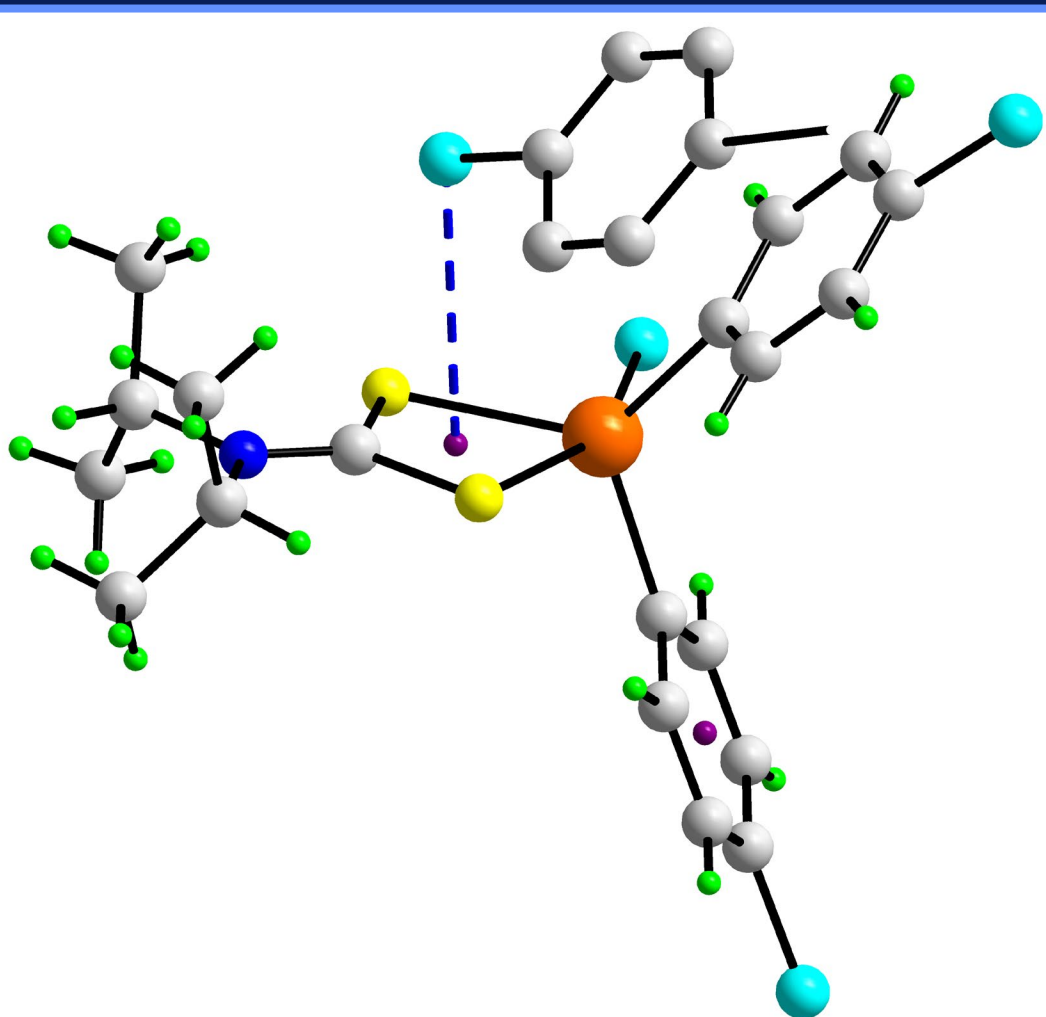


(a)

(b)



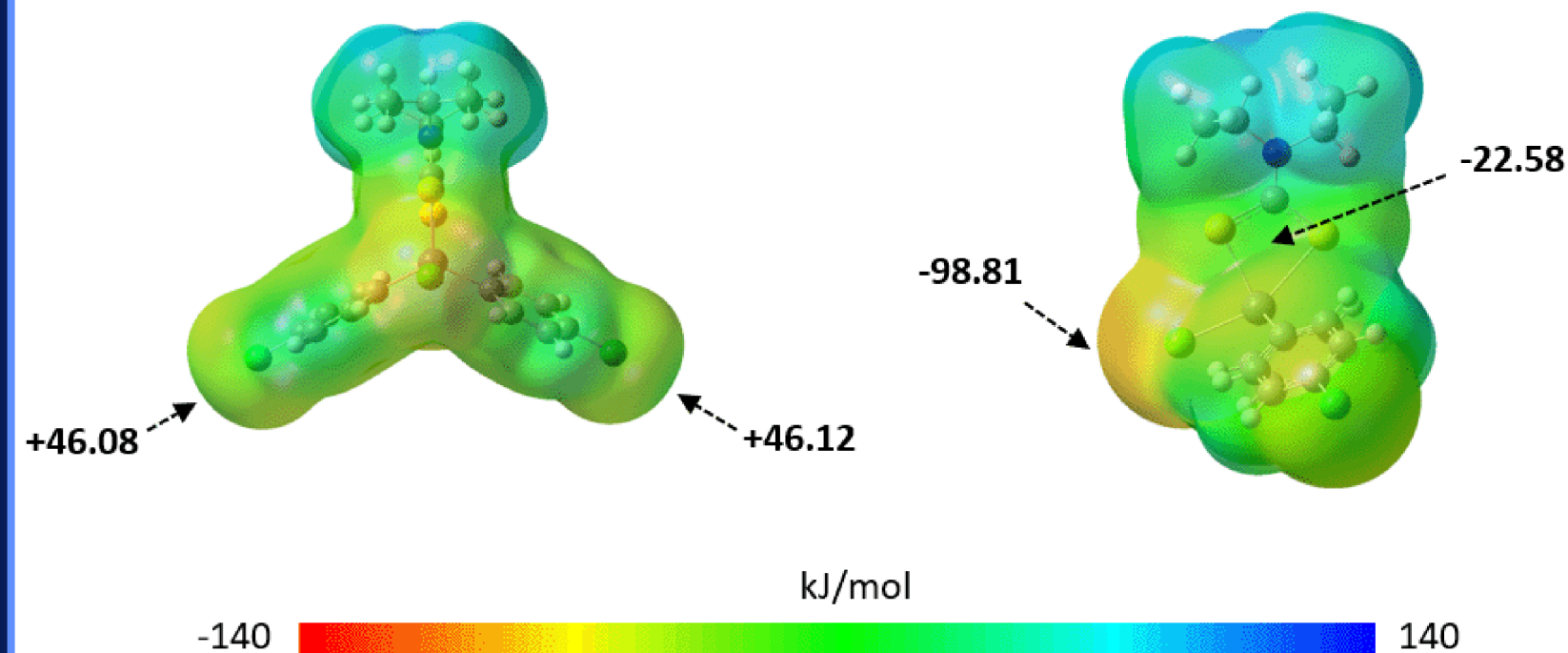
C-Cl... π (chelate ring) interaction



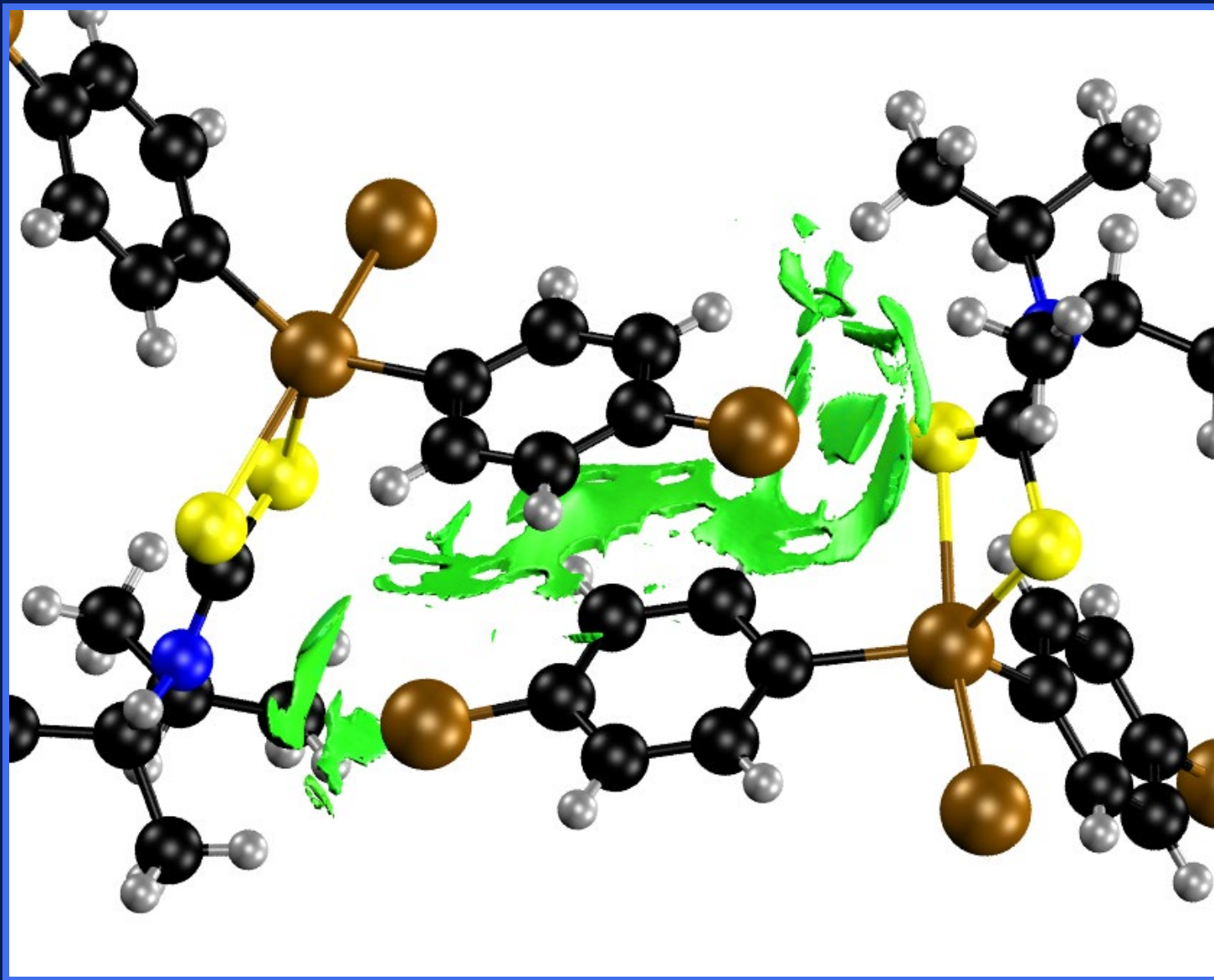
	sep. (Å)	vdW (Å)
Cl...Sn	4.35	3.95
Cl...S	3.94	3.55
Cl...S	3.77	3.55
Cl...C	3.61	3.45

MEPS

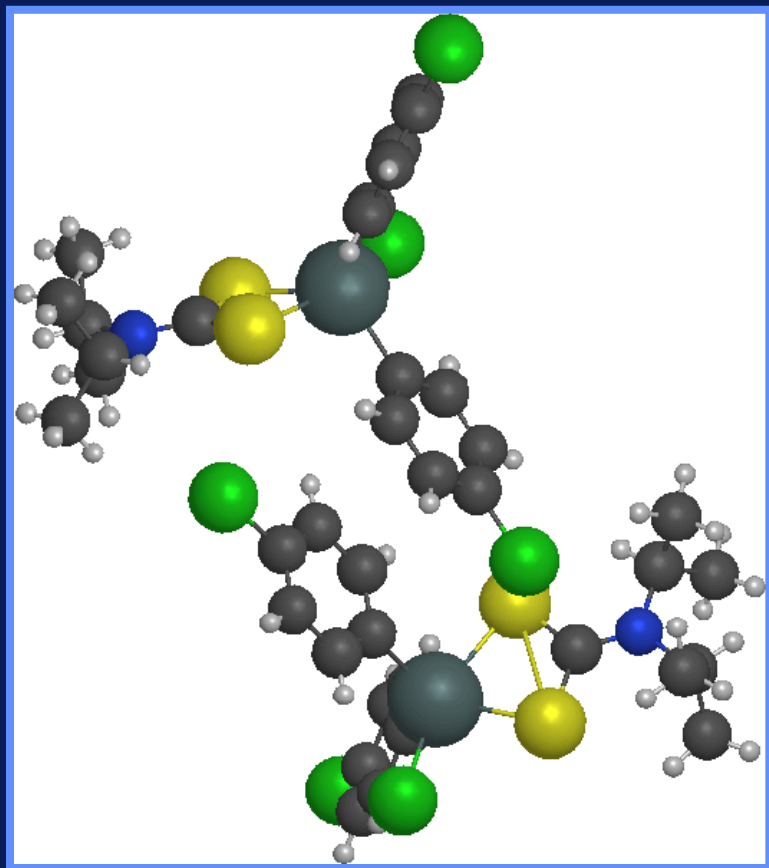
Alan Tan



Non-covalent Interaction plots



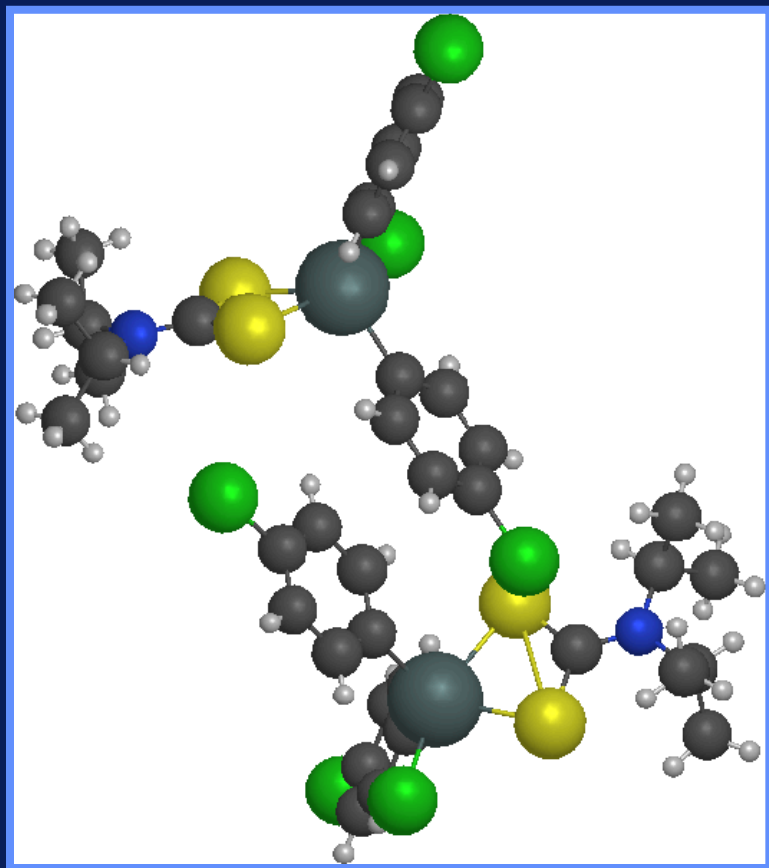
Binding energy



**Alberto
Otero-de-la-Roza**

12.22 kcal/mol

Binding energy

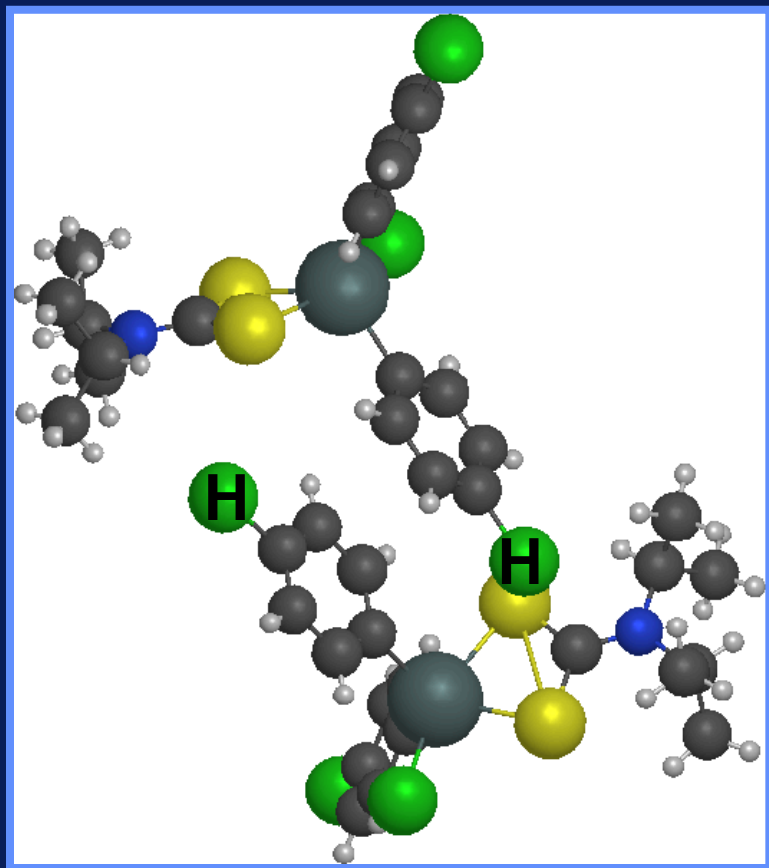


**Alberto
Otero-de-la-Roza**

12.22 kcal/mol

$\pi \cdots \pi$ 2-10 kcal/mol

Binding energy



12.2 kcal/mol

Replace both Cl with H

7.2 kcal/mol

2.5 kcal/mol per $\text{Cl}\cdots\pi$

cf. 1.5-2.8 kcal/mol $\text{C-H}\cdots\pi$

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Fortuna Eruditis Favet ("Fortune favours the prepared mind")